

Dimethyl adipate
627-93-0 | DTXSID8025096

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.95 | 0.69 | 0.95 | 0.65 | 0.96 | 0.68 |

Model Results

Predicted value: 4.75

Global applicability domain: Inside

Local applicability domain index: 9.25e-01

Confidence level: 8.86e-01

Nearest Neighbors from the Training Set

Image not found

Hexachloroethane

Measured: 4.47

Predicted: 4.45

Image not found

Pentyl ether

Measured: 4.80

Predicted: 4.98

Image not found

1,2,3-Trichlorobenzene

Measured: 5.19

Predicted: 5.00

Image not found

1,4-Dichlorobenzene

Measured: 4.46

Predicted: 4.45

Image not found

1,2,4-Trichlorobenzene

Measured: 4.95

Predicted: 5.06